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On the Processing of Thermal Scattering Law Data into ACE Format for Monte Carlo Transport Calculations

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ABSTRACT

Several codes for generating libraries for continuous energy Monte Carlo transport codes became available in recent years. The present work focuses on the preparation of thermal scattering law data with the ACEMAKER code in comparison with the NJOY code, which was the standard for many years. Scattering law data for hydrogen bound in zirconium hydride from the ENDF/B-VIII.0 library were chosen as an example. Performance of the processed data was tested on a set of benchmarks from the International Criticality Safety Benchmark Experiment Handbook. The results show the importance of the energy range to which thermal scattering law data are applied. A 0.3% tolerance for the construction of the input neutron energy grid and 32 equiprobable cosine bins were found to be sufficient for library preparation.

1 INTRODUCTION

In recent years several codes for producing application libraries from evaluated nuclear data files became available, in addition to NJOY [1], which is the standard code for producing libraries in ACE format for Monte Carlo transport calculations at the Los Alamos National Laboratory. A code verification exercise was conducted through the International Atomic Energy Agency (IAEA) to test the capabilities of codes to generate ACE libraries in the fast energy range [2]. The second phase of the exercise was initiated recently to test the capabilities of codes to process thermal scattering law data (TSL) into ACE_TSL format. The TSL of ZrH was chosen as an example. The test suite for testing the libraries was a set of criticality benchmarks from the International Criticality Safety Benchmark Experiment Project (ICSBEP). Different format options exist for representing the TSL data in the ACE_TSL files. In this work, the focus is on the ACEMAKER code [3], with which several sensitivity studies

were made. The results were found to be sensitive to the incident energy mesh by as much as 0.1% in k_eff due to data processing alone. The objective of this work is to provide some recommendations on the choice of processing options in generating ACE_TSL files.

2 CODE-VERIFICATION EXERCISE

In the past NJOY [1] was the only data processing system that could process evaluated nuclear data libraries in ENDF-6 format [4] into ACE library format for use with continuous-energy Monte Carlo transport codes, such as MCNP [5], Serpent [6], OpenMC [7] and others. The NJOY code was not generally available, so the users in member states of the International Atomic Energy Agency (IAEA) requested support to provide a freely available code for generating application libraries in ACE format. A project was initiated to develop the ACEMAKER code for the task. In the meantime, several other research groups also produced their own data processing codes, and NJOY became an open-source code, freely available to everyone. Nevertheless, having the choice of several codes for the same task allows inter-comparison and helps to identify and remove errors. The codes and authors that participated in the first phase of the code verification process that addressed the so-called "fast" ACE files (covering the energy range above thermal) were the following: NJOY (USA), FUDGE (USA), GRUCON (Russia), FRENDY (Japan), ACEMAKER/PREPRO (IAEA), GAIA (France), GALILEE (France), RULER (China), NECP-Atlas (China). Detailed references to the codes can be found in the summary document from the Meeting [8].

Code inter-comparison exercise allowed the developers to make some improvements to their codes. At the end, all participating codes successfully passed the test of cross-section linearization, resonance reconstruction, Doppler-broadening, and self-shielding. Some of the codes relied on the ACER module of NJOY for the final assembly of the ACE files. However, the first stage of the exercise addressed only the energy region above thermal. Problems exhibiting a significant amount of thermalization require data for the moderating materials in the so-called ACE-TSL format to describe scattering events at thermal neutron energies. The second phase of the code verification exercise was initiated at the IAEA to test the capabilities of the codes to process thermal scattering law data (TSL). A Meeting is planned in Autumn 2021 to review the current status of different codes.

3 THE ACEMAKER PACKAGE

The ACEMAKER-2.0 package [3] is a system of modules that makes use of the processing capabilities of the ENDF Pre-Processing codes [9, 10] available from the IAEA for preparing linearly interpolable cross-section data at any temperature and linearly interpolable angular or energy distributions. Furthermore, it includes its own capabilities to process coupled angle/energy distributions and re-formats all required data in the ACE format for energies above thermal (fast region). Moreover, ACEMAKER-2.0 also includes the module DOTSL to process the thermal scattering law (TSL) data for generating a thermal ACE-formatted file for Monte Carlo simulations. Processing of the TSL data is done independently of any other data processing modules.

Evaluated nuclear data formats and procedures for TSL are presented in Ref. [4]. The DOTSL processing methods are explained in Ref [3]. Here a brief description of the main options used for the case of H and Zr bound in ZrH is given for the sake of completeness.

The inelastic thermal scattering data are prepared from the evaluated nuclear data given in the section MF7/MT4 for S(α,β, T). The double differential inelastic cross-section at temperature *T*, $\sigma_{ine}(E \rightarrow E', \mu, T)$, for the main scattering atom can be calculated as:

$$\sigma_{ine}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S(\alpha, \beta, T) \quad (1)$$

where *E* is the incident neutron energy, *E'* is the outgoing energy of the scattered neutron, μ is the scattering cosine in the laboratory system, σ_b is the characteristic bound inelastic cross-section, *k* is the Boltzmann's constant, β is the dimensionless energy transfer and α is the dimensionless momentum transfer.

The thermal scattering law $S(\alpha,\beta,T)$ describes the binding of the scattering atom in a material and is tabulated as a function of α, β and *T* in section MF7/MT4 of an ENDF file. If the values of α or β are outside the range of the table, the differential scattering cross section can be computed using the short collision time (SCT) approximation

$$\sigma_{ine}^{SCT}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\left(4\pi\alpha\frac{T_{eff}}{T}\right)^{-\frac{1}{2}}e^{-\frac{(\alpha-|\beta|)^2\,T_{eff}}{4\alpha\quad T}-\frac{\beta+|\beta|}{2}} \quad (2)$$

where T_{eff} is the effective temperature, which is included in the evaluated nuclear data file.

The following steps need to be completed for preparing the inelastic ACE-formatted data at the requested temperature *T*:

1. The generation of a dense incident energy (*E*) grid: DOTSL generates an incident energy grid in such a way that a cross section that follows a "1/E" behavior can be linearly interpolated within a fractional tolerance given by:

$$tol = \begin{cases} 2.0 \cdot tolin & for \quad E_{min} \le E \le 0.0001\ eV \\ tolin & for \quad 0.0001 \le E \le 0.001\ eV \\ 0.5 \cdot tolin & for \quad 0.001 \le E \le 2.0\ eV \\ tolin & for \quad 2.0 \le E \le E_{max}\ eV \end{cases} \quad (3)$$

where $tolin = \min(TOLE, 0.001)$, and TOLE is the input parameter related to the tolerance of the function on the incident energy grid.

2. The adaptive generation of the outgoing energy grid to calculate $\sigma_{ine}(E \rightarrow E')$ and N_u equiprobable cosines $\bar{\mu}_i^{ine}(E, E')$: DOTSL prepares an initial outgoing particle energy grid for each incident energy *E* from the β values given in the $S(\alpha,\beta)$ tabulation, applying the restriction $E' \geq 0.0\ eV$. Then, each *E'* interval is further subdivided by successive halving until the value of $\sigma_{ine}(E \rightarrow E')$ and the N_u equiprobable cosines $\bar{\mu}_i^{ine}(E, E')$ can be linearly interpolated to within the tolerance TOL, which is as also an input parameter. Once the outgoing energy grid has been constructed the inelastic cross-section $\sigma_{ine}(E)$ is calculating by integration of $\sigma_{ine}(E \rightarrow E')$, using the trapezoid rule.
3. The adaptive generation of the cosine grid: DOTSL adaptively builds a cosine grid to compute the integral of $\sigma_{ine}(E \rightarrow E', \mu)$ and the equally probable cosines $\bar{\mu}_i^{ine}(E, E')$. An initial cosine grid is prepared for each value of the incident energy *E* and the ongoing energy E' from the values of α supplied in the $S(\alpha,\beta)$ tabulation, considering the restriction $-1.0 \le \mu \le 1.0$. Then, each μ interval is subdivided by successive halving until the energy angular distribution $\sigma_{ine}(E \rightarrow E', \mu)$ can be linearly interpolated to within the

specified tolerance. After that, the values of $\sigma_{ine}(E \rightarrow E')$ and $\overline{\mu}_i^{ine}(E, E')$ are calculated.

4. Thinning of the dense incident energy grid: A thinning procedure is applied in such a way that the incident energy *E* is removed if the cross-sections $\sigma_{ine}(E)$ and the average cosines $\overline{\mu}_i^{ine}(E)$ are linearly interpolable from the adjacent energy points within the input tolerance TOLE. The thinning algorithm tries to keep the shape of the functions as far as possible.
5. Calculation of the probability density function $PDF(E, E')$ and the cumulative density function $CDF(E, E')$ from $\sigma_{ine}(E \rightarrow E')$ and $\sigma_{ine}(E)$.
6. Thinning of the outgoing energy grid for each selected incident energy *E*: The data at outgoing energy *E'* are removed if the differences in the cumulative $CDF(E, E')$ and in the average cosine $\bar{\mu}^{ine}(E, E')$ with respect to the last selected *E'* are less than 0.000001 and 0.00625 respectively.

For H and Zr bound in ZrH the elastic scattering (*E*=*E'*) shows an incoherent component, therefore according to the ENDF-6 format manual [4] the differential cross section is given by:

$$\sigma_{ela}^{inc}(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2} e^{-2EW'(T)(1-\mu)} \delta(E - E') \tag{4}$$

where σ_b is the characteristic bound cross section [barns], *W'* is the Debye-Waller integral divided by atomic mass [eV^{-1}] and all the other symbols have the same meaning as above.

The values of σ_b and *W'* can be obtained from section MF7/MT2 of an ENDF-6 formatted evaluation. The integral incoherent elastic cross section $\sigma_{ela}^{inc}(E)$ and the equally probable cosines $\bar{\mu}_i^{inc}(E)$ are analytically obtained by:

$$\sigma_{ela}^{inc}(E) = \frac{\sigma_b}{2}\left(\frac{1 - e^{-4W'E}}{2EW'}\right) \tag{5}$$

$$\mu_i^{inc}(E) = 1 + \frac{1}{2W'E} ln\left\{\frac{1 - e^{-4W'E}}{N_u} + e^{-2W'E\left[1-\mu_{i-1}^{inc}(E)\right]}\right\} \tag{6}$$

$$\bar{\mu}_i^{inc}(E) = \frac{N_u}{2W'E}\left\{\frac{\left[2W'E\mu_i^{inc}(E) - 1\right]e^{-2W'E[1-\mu_i^{inc}(E)]} - \left[2W'E\mu_{i-1}^{inc}(E) - 1\right]e^{-2W'E[1-\mu_{i-1}^{inc}(E)]}}{1 - e^{-4W'E}}\right\} \tag{7}$$

where $\mu_i^{inc}(E)$ represents the upper boundary of the equally probable interval *I,* with $i = 1,2,3, \ldots N_u$ and $\mu_0^{inc}(E) = -1$. The incident energy grid of the inelastic scattering is used to compute $\sigma_{ela}^{inc}(E)$. A thinning algorithm similar as describe above is applied to reduce the number of incident energies.

4 RESULTS

4.1 Benchmark suite

Data processing was tested on the thermal scattering law data of zirconium hydride. TSL of hydrogen in ZrH and Zr in ZrH are available in the ENDF/B-VIII.0 library. A selection of benchmark cases from the ICSBEP handbook that involve ZrH is given in Table 1.

Table 1: List of benchmark cases containing ZrH

No.	ICSBEP Label	Short name	Common name	Comment
1	HEU-COMP-MIXED-003	hcm003-001	Narcis-M-1	ZrH moderator
2	HEU-COMP-THERM-007	hct007-004	RRCt-1(cyl)	U-Cu/ZrH SS_clad
3	HEU-COMP-THERM-007	hct007-005	RRCt-2(cyl)	U-Cu/ZrH SS_clad
4	HEU-COMP-THERM-007	hct007-006	RRCt-3(cyl)	U-Cu/ZrH SS_clad
5	IEU-COMP-THERM-003	ict003-001	TRIGA	SS_clad(ZrH)
6	IEU-COMP-THERM-003	ict003-002	TRIGA	SS_clad(ZrH)
7	IEU-COMP-THERM-013	ict013-001	NRAD_TRIGA_56	ZrH Er U(20%)
8	IEU-COMP-THERM-013	ict013-002	NRAD_TRIGA_60	ZrH Er U(20%)
9	IEU-COMP-THERM-013	ict013-003	NRAD_TRIGA_62	ZrH Er U(20%)
10	IEU-COMP-THERM-013	ict013-004	NRAD_TRIGA_64	ZrH Er U(20%)

4.2 Sensitivity studies

To study the impact of various parameters on the calculated reactivity the benchmark case "ict013-001" was taken as an example.

Calculations with NJOY were done for different numbers of cosine bins and for different upper energies of TSL. Note that the $S(\alpha,\beta)$ data in the ENDF/B-VII.0 library only go up to 1.973 eV; due to the fixed energy grid in NJOY the upper energy for $S(\alpha,\beta)$ is effectively rounded to1.855 eV. Above this energy the "Short collision time" approximation (SCT) is used up to the energy nearest to the specified energy for TSL, which is 3.75 eV when 4 eV is specified as the limit. At higher energies the free-gas approximation is applied.

The ACEMAKER code treats the TSL data using adaptive energy grid. This means that the $S(\alpha,\beta)$ data are treated properly up to 1.973 eV and the SCT approximation is used up to the specified upper thermal energy. ACEMAKER calculations were done with 64, 48, 32, 20 and 16 cosines bins. The upper energy was 4 eV in all cases and the tolerance for preparing the incident energy grid were 0.05%, 0.1%, 0.2%, 0.5% and 1.0%. The statistical uncertainty in the MCNP calculations was generally close to 5 pcm (parts per 100 000). The results are shown in Table 2.

Table2 : k_eff for the ICT013 benchmark using different TSL processing options

Code	Ncos	Etop[eV]	Tol.[%]	Points Inelastic	Points Elastic	k_eff	dk[pcm]	Size
NJOY Original	20	1.855	-	98	98	1.01294	31	2 605 690
NJOY	20	1.855	-	98	98	1.01296	33	2 605 690
	20	3.75	-	106	106	1.01262	-1	2 980 499
	32	3.75	-	106	106	1.01263	0	4 558 580
	64	3.75	-	106	106	1.01273	10	8 831 188
ACEMAKER	64	4.0	0.10	196	167	1.01263	Ref.	18 412 085
	64	4.0	0.20	154	101	1.01266	3	14 591 777
	64	4.0	0.30	119	94	1.01265	2	11 514 334
	64	4.0	0.50	109	62	1.01256	-7	10 585 371
	64	4.0	1.00	82	41	1.01265	2	8 168 527
	64	4.0	1.50	73	31	1.01257	-6	7 345 004
	48	4.0	0.10	196	167	1.01257	-6	13 999 456
	32	4.0	0.10	196	167	1.01260	-3	9 589 814
	20	4.0	0.10	196	167	1.01257	-6	6 282 357
	16	4.0	0.10	196	167	1.01255	-8	5 182 166

4.3 Results and discussion

Table 2 shows the results of MCNP calculations for the ICT013-001 benchmark. The first two rows show that the result with a locally-generated ACE file with NJOY2016 is practically equal to the one with the original ACE-TSL library available from LANL. The next three rows show that the impact of using the SCT approximation up to 3.75 eV, which amounts to 34 pcm difference from the reference ACEMAKER result with the tightest data reconstruction tolerances. The result is practically independent of the number of cosine bins. There is a relatively modest increase in the number of points in the incident energy grid by extending the TSL energy range to 3.75 eV, and correspondingly in the file size, governed by the allocated storage array length. On the contrary, the increase in the file size due to a larger number of cosine bins is very large, with a modest impact on the calculated multiplication factor. The incident neutron energy grid in NJOY is hard-coded and cannot be changed. The ACEMAKER code is more flexible in this respect. The number of points depends on the requested reconstruction tolerance requested on input. Calculations were done using different reconstruction tolerances, as well as different numbers of cosine bins. Taking the first ACEMAKER result with tightest data reconstruction tolerances as reference, the results in Table 2 lead us to conclude that a 0.3% tolerance and 32 cosine bins is a reasonable compromise in terms of the file size for generating the ACE-TSL files for H in ZrH.

Full scale calculations for the selected benchmarks listed in Table 1 were performed using the original ACE-TSL library based on ENDF/B-VIII.0 and the ACE-TSL files for H in ZrH and Zr in ZrH produced with ACEMAKER with 0.3% tolerance and 32 cosine bins (label "e80_ACEM9_t003b32"). The results are practically the same as those obtained with 0.1% tolerance and 64 cosine bins (label "e80_ACEM9_t001"). The results are displayed graphically in Fig.1. The Narcis-M1 benchmark has no uncertainty specified. The NRAD-TRIGA benchmarks are strongly discrepant, indicating a possible problem with benchmark specifications or nuclear data, but the problem is not related to the nuclear data processing.

5 CONCLUSIONS

Data processing options were investigated on the example of thermal scattering law data for hydrogen in zirconium hydride data in the ACE-TSL files based on the ENDF/B-VIII.0 library. Full scale calculations for the selected benchmarks were performed using the original ACE-TSL library and the ACE-TSL files produced with the ACEMAKER code with 0.3% tolerance for generating the incident neutron energy grid and 32 cosine bins. The results show considerable dependence on the upper energy to which the TSL data are applied, which suggests that on re-evaluation of the TSL data the $S(\alpha,\beta)$ grid should be extended to higher energies. The grid density affects the size of the ACE-TSL file. Calculations show that a 0.3% reconstruction tolerance and 32 cosine bins are sufficient to describe the thermal scattering law of H in ZrH.

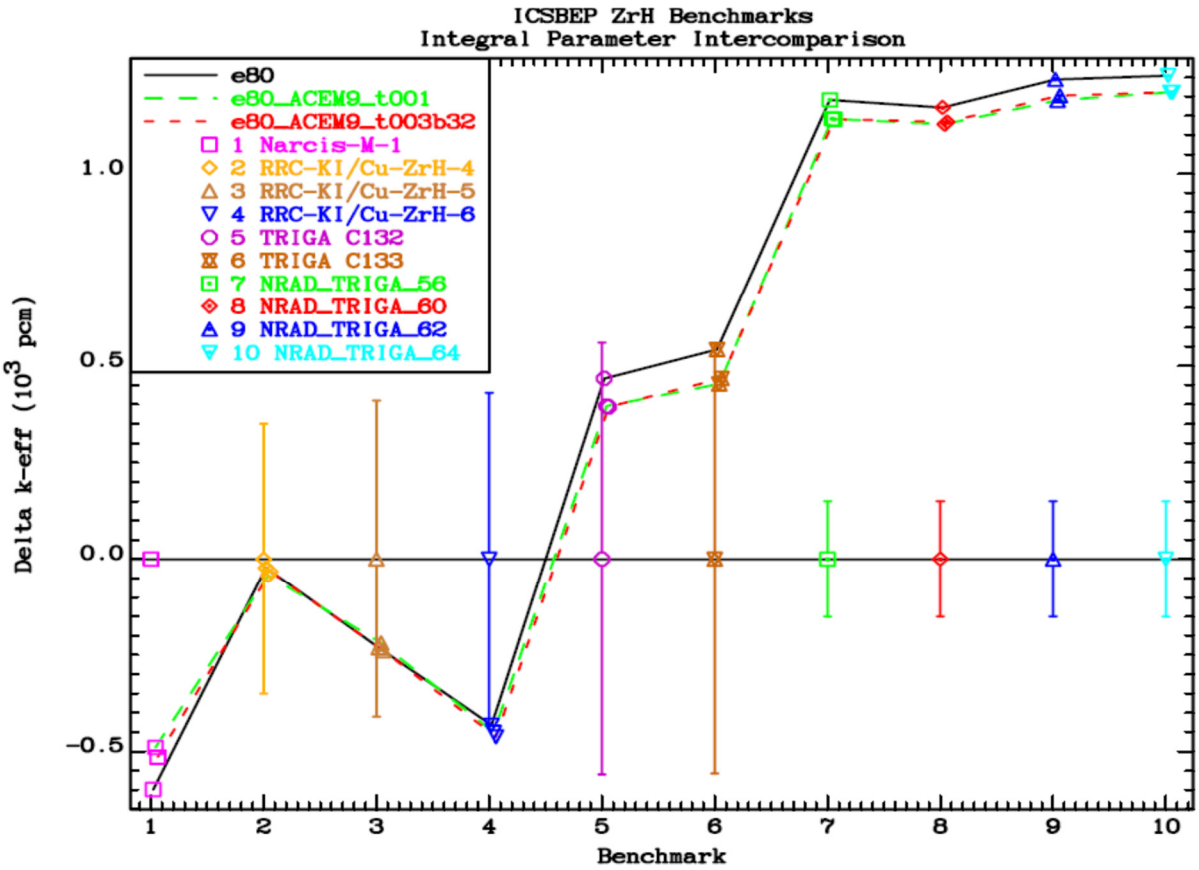

Figure 1: Comparison of the results for ZrH benchmarks with TSL-ACE files prepared by NJOY (label "e80") and by ACEMAKER (label "e80_ACEM9_t001" and "e80_ACEM9_t003b32"), respectively. The lines are eyeguides for easier distinction between the results.

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